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ON BOUNDING EXACT MODELS OF EPIDEMIC SPREAD ON NETWORKS

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ABSTRACT. In this paper we use comparison theorems from classical ODE theory in order to rigorously show that closures or approximations at individual or node level lead to mean-field models that bound the exact stochastic process from above. This will be done in the context of modelling epidemic spread on networks and the proof of the result relies on the observation that the epidemic process is negatively correlated (in the sense that the probability of an edge being in the susceptible-infected state is smaller than the product of the probabilities of the nodes being in the susceptible and infected states, respectively). The results in the paper hold for Markovian epidemics and arbitrary weighted and directed networks. Furthermore, we cast the results in a more general framework where alternative closures, other than that assuming the independence of nodes connected by an edge, are possible and provide a succinct summary of the stability analysis of the resulting more general mean-field models. While deterministic initial conditions are key to obtain the negative correlation result we show that this condition can be relaxed as long as extra conditions on the edge weights are imposed.

1. Introduction. Modelling transmission processes on networks, such as epidemics and rumours, has led to many mathematical challenges [22, 12]. This is mainly due to the high dimensionality of the exact model, which is often a continuous time Markov chain where the size of the state space scales as m^N , where m is the number of states a node can be in and N is the number of nodes in the network [27, 30]. While theoretically the master equations can be given, their rigorous analysis is out of reach due to the high dimensionality. One approach to deal with this challenge is to consider some ‘clever’ averaging, at node or at population level, and proceed to derive evolution equations for some newly defined average quantities. These however, more often than not, depend on other new average quantities which are of higher order, e.g. the expected number of nodes in a certain state usually depends

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on the expected number of links/edges in certain states. As a rule of thumb, the dependency between moments is broken by making some closure assumptions where higher order moments are approximated by lower-order ones. This then leads to a low-dimensional system of ordinary differential equations (integro-differential and delay differential equations are also possible) or mean-field model.

The approach above has led to a myriad of mean-field models for *SIS* (susceptible-infected-susceptible) and *SIR* (susceptible-infected-recovered) epidemics which are able to capture the average behaviour of epidemics on certain network types (e.g. tree networks and networks build using the configuration model). The most well-known such models are: (a) heterogenous degree-based [23, 6], (b) pairwise [24, 11, 4, 27, 30, 14], (c) effective-degree [17], (d) edge-based compartmental [18, 19], (e) pair-based [25, 26, 13] and (f) N-Intertwined Mean-Field Approximation (NIMFA) [32, 31]. When such models perform well, i.e. output from these agrees well with results from the exact or simulation model, one can proceed to analyse them and to derive analytical results concerning the epidemic threshold and final size, or quasi-equilibrium for *SIS* epidemics. Such explicit relations between network characteristics and spreading dynamics allow us to better understand how these factors interact and will ultimately lead to more efficient prevention and control measures.

In many cases, mean-field models are validated by simply comparing the results of explicit stochastic network simulation (which stands for the exact model) to output from mean-field models. Such tests are usually performed for a limited number of network types and combination of parameter values. While such heuristic arguments are useful, it is desirable that where possible the difference between the exact and mean-field models is rigorously established using sound mathematical arguments. This endeavour has already led to results proving that under some mild conditions on the degree distribution the edge-based compartmental model is exact for *SIR* epidemics in the limit of large networks built based on the configuration model [20]. In the case of *SIS* propagation on a complete graph or on a regular random network the model is a density dependent Markov chain and functional analytic tools can be used to prove that the difference between the output of the mean-field and the exact system scales as $1/N$ for large system size N [5, 15]. Besides estimates on the difference, upper and lower bounds have also been derived for the prevalence obtained from the exact model when *SIS* or *SIR* propagation is considered on a complete graph, see [2, 1, 3]. These results are valid for graphs with very simple structure, motivating research for finding upper and lower bounds for more complex models.

In this paper, we focus on the NIMFA model for *SIS* epidemics and we will show that this model provides an upper bound on the exact model on arbitrary weighted and directed networks. In [32] it is claimed that the NIMFA model overestimates the prevalence obtained from the exact system, however, the rigorous proof is not presented there. Here, this is done by using some well-known results from the theory of differential inequalities. It is important to note that our results are not constrained to the NIMFA model since many other models make the assumptions that the state of nodes at the end of edges are independent and use this to close and generate a tractable model from an otherwise ungainly high-dimensional model. The paper is structured as follows. In Section 2 the exact model is formulated and a bottom-up approach is used. This means that the model starts at the level of nodes and focuses on the probability of nodes being either susceptible or infected. Also here, the closure at the level of pairs is generalised beyond simply assuming

that the state of nodes at the end of an edge are independent. In Section 3 the main result is presented and it is here where we rigorously prove that NIMFA provides an upper bound on the exact model. In Section 4 we show that negative correlations can be maintained even if starting from mixed initial conditions as long as extra conditions on the edges weights are imposed. This is followed by the analysis on the closed model in Section 5. The paper concludes with a short discussion of the main findings and possible extensions.

2. Model formulation. Consider a network with N nodes and assume that no node has an edge to itself, but we allow for node j to have an edge to node i having some weight g_{ij} . Typically $g_{ij} = 1$ if there is an edge from j to i and 0 otherwise, but the model formulation works for any directed and weighted network and thus we can consider $g_{ij} \in [0, \infty)$ for $i, j = 1, 2, \dots, N$. We can use the adjacency matrix $G = (g_{ij})_{i,j=1,2,\dots,N}$ to represent the network. We assume that the transmission rate from j to i is τg_{ij} . The recovery rate at each node is γ . The probability that node i is infected at time t is denoted by $\langle I_i \rangle(t)$. The aim is to derive exact and approximate differential equations for this function.

2.1. Exact model. It can be shown from first principles or from the exact master equations formulated in terms of the probabilities of all 2^N configurations [25] that $\langle I_i \rangle(t)$ satisfies the differential equation

$$\langle \dot{I}_i \rangle = \tau \sum_{j=1}^N g_{ij} \langle S_i I_j \rangle - \gamma \langle I_i \rangle, \quad (1)$$

where $\langle S_i I_j \rangle(t)$ is the probability that the pair consisting of node i and node j is of type $S - I$ at time t . This system is exact but not closed hence further differential equations or a closure is needed to determine the probability $\langle I_i \rangle(t)$. The differential equations for the pairs take the following form.

$$\langle \dot{S}_i I_j \rangle = \tau \sum_{k=1}^N g_{jk} \langle S_i S_j I_k \rangle - \tau \sum_{k=1}^N g_{ik} \langle I_k S_i I_j \rangle - \tau g_{ij} \langle S_i I_j \rangle - \gamma \langle S_i I_j \rangle + \gamma \langle I_i I_j \rangle, \quad (2)$$

$$\langle \dot{I}_i S_j \rangle = \tau \sum_{k=1}^N g_{ik} \langle I_k S_i S_j \rangle - \tau \sum_{k=1}^N g_{jk} \langle I_i S_j I_k \rangle - \tau g_{ji} \langle I_i S_j \rangle - \gamma \langle I_i S_j \rangle + \gamma \langle I_i I_j \rangle, \quad (3)$$

$$\langle \dot{I}_i I_j \rangle = \tau \sum_{k=1}^N g_{jk} \langle I_i S_j I_k \rangle + \tau \sum_{k=1}^N g_{ik} \langle I_k S_i I_j \rangle - 2\gamma \langle I_i I_j \rangle + \tau g_{ij} \langle S_i I_j \rangle + \tau g_{ji} \langle I_i S_j \rangle, \quad (4)$$

$$\langle \dot{S}_i S_j \rangle = -\tau \sum_{k=1}^N g_{ik} \langle I_k S_i S_j \rangle - \tau \sum_{k=1}^N g_{jk} \langle S_i S_j I_k \rangle + \gamma \langle S_i I_j \rangle + \gamma \langle I_i S_j \rangle, \quad (5)$$

where $\langle A_i B_j C_k \rangle$ is the probability that the triple consisting of the nodes i, j and k is in the state $A - B - C$, and (i, j) runs over all pairs satisfying $1 \leq i < j \leq N$ and in all summations k is different from i and from j . Note that for any pair (i, j) we have that the right hand sides of the four differential equations sums to 0, that is the sum $\langle S_i I_j \rangle + \langle I_i S_j \rangle + \langle I_i I_j \rangle + \langle S_i S_j \rangle$ remains constant in time. If this constant is 1 at the initial time instant, then it remains 1 for all time.

	$\langle I_i \rangle$	$\langle S_i \rangle$	
$\langle I_j \rangle$	a	b	q
$\langle S_j \rangle$	c	d	1-q
	p	1-p	

TABLE 1. The relation of the joint and marginal probabilities.

2.2. Closure at the level of pairs. Closure at the level of pairs means that the joint probabilities $\langle S_i I_j \rangle$, $\langle I_i S_j \rangle$, $\langle I_i I_j \rangle$ and $\langle S_i S_j \rangle$ are expressed in terms of the marginal probabilities $\langle I_i \rangle$, $\langle I_j \rangle$, $\langle S_i \rangle$ and $\langle S_j \rangle$. This is always an approximation, as we will show below. However, we wish to rigorously quantify the accuracy of the approximation, or to be able to state whether a model based on closures gives upper or lower bounds for the exact values of the joint probabilities, or indeed if the prevalence from such a closed model is below or above the exact prevalence.

First we rigorously define what a closure relation means. The relation of the joint and marginal probabilities are shown in Table 1, where $a = \langle I_i I_j \rangle$, $b = \langle S_i I_j \rangle$, $c = \langle I_i S_j \rangle$ and $d = \langle S_i S_j \rangle$. All letters denote probabilities hence $a, b, c, d, p, q \in [0, 1]$. The marginals can be expressed in terms of the joint probabilities as

$$a + b = q = \langle I_j \rangle, \quad a + c = p = \langle I_i \rangle, \quad c + d = 1 - q, \quad b + d = 1 - p. \quad (6)$$

It can be immediately seen that $a + b + c + d = 1$, hence the four equations are not independent, therefore they cannot be solved for the unknowns a , b , c and d . This shows that the marginals do not determine the joint probabilities. However, once one of them is given then the remaining three are determined by system (6). A closure relation means that one of the joint probabilities is given by a certain algebraic relation involving the marginals, and the others are determined by system (6). Here we define the closure for the II pairs, i.e. a is specified in terms of p and q . (One can equivalently express the probabilities of SI , IS or SS pairs.) So a closure will be a function $W : [0, 1] \times [0, 1] \rightarrow [0, 1]$, for which

$$\langle I_i I_j \rangle \approx W(\langle I_i \rangle, \langle I_j \rangle).$$

In order to have a solution satisfying $a, b, c, d \in [0, 1]$, the function W must satisfy some conditions. On one hand, the first two equations of (6) show that $a \leq p$ and $a \leq q$ must hold, that is $a \leq \min(p, q)$. On the other hand, the third and fourth equations should give a nonnegative value for d , hence $1 - q - p + a \geq 0$ and $1 - p - q + a \geq 0$ must hold, leading to $\max(p + q - 1, 0) \leq a$. (The max operation is needed because $p + q - 1$ may be negative, when the lower bound for a is zero.) Finally, it is natural to assume that W is a symmetric function, i.e. $W(x, y) = W(y, x)$, leading to the following definition of the closure.

Definition 2.1. A symmetric function $W : [0, 1] \times [0, 1] \rightarrow [0, 1]$ is called a closure relation if

$$\max(x + y - 1, 0) \leq W(x, y) \leq \min(x, y) \text{ for all } x, y \in [0, 1].$$

We note that the most important closure relation is $W(x, y) = xy$ leading to the solution of system (6) in the form

$$a = pq, \quad b = (1 - p)q, \quad c = p(1 - q), \quad d = (1 - p)(1 - q).$$

This corresponds to the case when the states of node i and j are independent, i.e. the joint probability is the product of the marginals. To check that $W(x, y) = xy$

satisfies the inequalities in the definition is an easy exercise and is left to the reader. One can also immediately see that $W(x, y) = \min(x, y)$ and $W(x, y) = \max(x + y - 1, 0)$ are proper closure relations.

Once a closure relation is chosen, the closed form of (1) can be given as follows. Since $W(\langle I_i \rangle, \langle I_j \rangle)$ gives an approximation of $\langle I_i I_j \rangle$ and $\langle S_i I_j \rangle + \langle I_i I_j \rangle = \langle I_j \rangle$, one can approximate $\langle S_i I_j \rangle$ as $\langle I_j \rangle - W(\langle I_i \rangle, \langle I_j \rangle)$. Hence the closed system is

$$\dot{X}_i = \tau \sum_{j=1}^N g_{ij}(X_j - W(X_i, X_j)) - \gamma X_i. \quad (7)$$

Solving this system for X_i yields an approximation for $\langle I_i \rangle$.

The ‘art’ of closing (1) lies in choosing W in a way in which X_i is as close as possible to $\langle I_i \rangle$. In fact, the only function used in the literature is $W(x, y) = xy$ and the accuracy of the closure has been investigated only numerically. Here our goal is slightly different. We want to find upper and lower bounds to $\langle I_i \rangle$, i.e. to introduce closures w and W in such a way that for the corresponding solutions x_i and X_i of (7) the inequalities

$$x_i \leq \langle I_i \rangle \leq X_i$$

hold.

We will show that $W(x, y) = xy$ gives an upper bound and $W(x, y) = \min(x, y)$ gives a lower bound. However, improving these bounds by more sophisticated closures remains an open question. First, in the next section, we derive conditions on the closure W ensuring that (7) gives an upper or lower bound.

3. Bounds for the exact system. The derivation of the upper bound is based on the fact that $S - I$ pairs are non-negatively, and $I - I$ and $S - S$ pairs are non-positively correlated [7], that is we have for any i and j that

$$\langle S_i I_j \rangle \leq \langle S_i \rangle \langle I_j \rangle, \quad \langle I_i I_j \rangle \geq \langle I_i \rangle \langle I_j \rangle, \quad \langle S_i S_j \rangle \geq \langle S_i \rangle \langle S_j \rangle. \quad (8)$$

To be precise, in [7] the authors proved that the above inequality holds as long as the initial condition is deterministic, i.e. the epidemic at time $t = 0$ starts from one of the 2^N states with probability one, the infectious and recovery processes are Markovian and the weights or infectious rates across edges are arbitrary positive numbers. Their result is based on a graphical construction introduced in [8], which is widespread in the interacting particle processes literature. While in Section 4 we make further remarks on correlations and provide some results based on an ODE-based approach, here we will use the result in [7] to give an upper bound for the solution of system (1). The latter is done below. The first relation leads to the differential inequality

$$\dot{\langle I_i \rangle} \leq \tau \sum_{j=1}^N g_{ij} \langle S_i \rangle \langle I_j \rangle - \gamma \langle I_i \rangle. \quad (9)$$

Based on this inequality let us introduce the following system of differential equations, called individual-based model or N-intertwined mean-field approximation (NIMFA) [32, 31].

$$\dot{Y}_i = \tau \sum_{j=1}^N g_{ij}(1 - Y_i)Y_j - \gamma Y_i. \quad (10)$$

Since we have the same right hand side in (9) and (10) with inequality in the first, we expect that the NIMFA approximation yields an upper bound on the exact

solution. We will prove this by using the comparison theory of ODEs based on the Kamke-Müller condition which is detailed below.

Consider the ODE $\dot{x}(t) = f(x(t))$ and the differential inequality $\dot{y}(t) \leq f(y(t))$ with a given differentiable function $f : \mathbb{R}^n \rightarrow \mathbb{R}^n$ subject to initial conditions satisfying $y(0) \leq x(0)$. The aim is to find conditions on f ensuring that $y(t) \leq x(t)$ for $t \geq 0$. In what follows, the ordering relation for vectors is used in the following sense:

$$u \leq v, \text{ if } u_i \leq v_i \ \forall i = 1, 2, \dots, n, \quad u < v, \text{ if } u_i < v_i \ \forall i = 1, 2, \dots, n.$$

A sufficient condition on f for the desired inequality to hold is the Kamke-Müller condition [10, 21], which is equivalent to requiring that

$$\text{if } u \leq v \text{ and } u_i = v_i \text{ for some } i \in \{1, 2, \dots, n\} \Rightarrow f_i(u) \leq f_i(v).$$

This condition essentially means that the function in the i -th coordinate, f_i is increasing in all coordinates x_j for $j \neq i$. However, this leads to an alternative sufficient condition, which if satisfied, allows us to call the f function cooperative. More precisely, f is called cooperative if

$$\partial_j f_i \geq 0 \ \forall i, j = 1, 2, \dots, n \text{ and } i \neq j.$$

It can be shown that if f is cooperative in a convex domain, then it satisfies the Kamke-Müller condition. A detailed and comprehensive study of differential inequalities and comparison theory can be found in the book by Szarski [29]. Cooperative systems generate monotone dynamical systems that are dealt with in the book chapter by Hirsch and Smith [9] and the book by Smith [28]. The main comparison result used here is the following.

Lemma 3.1. *Assume that f satisfies the Kamke-Müller condition. If $\dot{x}(t) = f(x(t))$ and the differential inequality $\dot{y}(t) \leq f(y(t))$ holds for $t \geq 0$ and $y(0) \leq x(0)$, then $y(t) \leq x(t)$ for all $t \geq 0$.*

Using this comparison result we can derive the following theorems about the upper and lower bounds.

Theorem 3.2. *Consider a weighted and directed network G , the exact individual-based SIS model given by system (1) and the closed system (7) with a closure W satisfying (besides the conditions in Definition 2.1)*

- (i) $y \mapsto y - W(x, y)$ is an increasing function,
- (ii) $\langle I_i I_j \rangle \geq W(\langle I_i \rangle, \langle I_j \rangle)$ for all i, j .

Assuming that both models start with identical initial conditions, $\langle I_i \rangle(0) = X_i(0)$ ($i = 1, 2, \dots, N$), it follows that $\langle I_i \rangle(t) \leq X_i(t) \ \forall i = 1, 2, \dots, N$ and $\forall t \geq 0$.

PROOF. We start from the exact system,

$$\begin{aligned} \dot{\langle I_i \rangle} &= \tau \sum_{j=1}^N g_{ij} \langle S_i I_j \rangle - \gamma \langle I_i \rangle = \tau \sum_{j=1}^N g_{ij} (\langle I_j \rangle - \langle I_i I_j \rangle) - \gamma \langle I_i \rangle \\ &= \tau \sum_{j=1}^N g_{ij} (\langle I_j \rangle - W(\langle I_i \rangle, \langle I_j \rangle)) - \gamma \langle I_i \rangle + \tau \sum_{j=1}^N g_{ij} (W(\langle I_i \rangle, \langle I_j \rangle) - \langle I_i I_j \rangle) \\ &\leq \tau \sum_{j=1}^N g_{ij} (\langle I_j \rangle - W(\langle I_i \rangle, \langle I_j \rangle)) - \gamma \langle I_i \rangle, \end{aligned} \tag{11}$$

where we have used (ii). The right-hand side of the closed system (7) can be given by the function $f : \mathbb{R}^N \rightarrow \mathbb{R}^N$ with coordinate functions

$$f_i(x) = \tau \sum_{j=1}^N g_{ij}(x_j - W(x_i, x_j)) - \gamma x_i.$$

It can immediately be seen that the solution of the closed system satisfies the differential equation $\dot{x}(t) = f(x(t))$, and the solution of the exact system satisfies the differential inequality $\dot{y}(t) \leq f(y(t))$, with both systems starting from the same initial condition. According to (i) the coordinate function f_i is increasing in the variable x_j , hence f satisfies the Kamke-Müller condition. Therefore, the general comparison Lemma 3.1 implies that $\langle I_i \rangle(t) \leq X_i(t) \forall i = 1, 2, \dots, N$ and $\forall t \geq 0$.

□

Now, using the closure $W(x, y) = xy$ we can prove that (10) gives an upper bound. Namely, we have seen that $W(x, y) = xy$ satisfies the conditions in Definition 2.1. Moreover, $y - xy = y(1 - x)$ is increasing in y when $x \in [0, 1]$, that is (i) holds. In Section 4 we will prove that (ii) also holds, hence $W(x, y) = xy$ satisfies the conditions of Theorem 3.2 leading to the following corollary.

Corollary 1. *Consider a weighted and directed network G , the exact individual-based SIS model given by system (1) and the individual-based closed system (10). Assuming that both models start with identical initial conditions, $\langle I_i \rangle(0) = Y_i(0)$ ($i = 1, 2, \dots, N$), it follows that $\langle I_i \rangle(t) \leq Y_i(t) \forall i = 1, 2, \dots, N$ and $\forall t \geq 0$.*

Similarly to Theorem 3.2, the following result can be proved about the lower bound.

Theorem 3.3. *Consider a weighted and directed network G , the exact individual-based SIS model given by system (1) and the closed system (7) with a closure W satisfying (besides the conditions in Definition 2.1)*

- (i) $y \mapsto y - W(x, y)$ is an increasing function,
- (ii) $\langle I_i I_j \rangle \leq W(\langle I_i \rangle, \langle I_j \rangle)$ for all i, j .

Assuming that both models start with identical initial conditions, $\langle I_i \rangle(0) = X_i(0)$ ($i = 1, 2, \dots, N$), it follows that $\langle I_i \rangle(t) \geq X_i(t) \forall i = 1, 2, \dots, N$ and $\forall t \geq 0$.

It is easy to see that $W(x, y) = \min(x, y)$ satisfies the assumptions of the theorem. Namely, we have seen that $W(x, y) = \min(x, y)$ satisfies the conditions in Definition 2.1. Moreover, $y - \min(x, y) = \max(y - x, 0) = \frac{1}{2}(|y - x| + y - x)$ is increasing in y , that is (i) holds. In the previous section we saw that $\langle I_i I_j \rangle \leq \langle I_i \rangle$ and $\langle I_i I_j \rangle \leq \langle I_j \rangle$, hence (ii) also holds. Thus $W(x, y) = \min(x, y)$ satisfies the assumptions of Theorem 3.3 leading to the following corollary.

Corollary 2. *Consider a weighted and directed network G , the exact individual-based SIS model given by system (1) and the individual-based closed system*

$$\dot{X}_i = \tau \sum_{j=1}^N g_{ij}(X_j - \min(X_i, X_j)) - \gamma X_i. \quad (12)$$

Assuming that both models start with identical initial conditions, $\langle I_i \rangle(0) = X_i(0)$ ($i = 1, 2, \dots, N$), it follows that $\langle I_i \rangle(t) \geq X_i(t) \forall i = 1, 2, \dots, N$ and $\forall t \geq 0$.

4. Remarks on the correlation of $S - I$ pairs. In this section we focus on the inequalities in (8) and look at relaxing the assumption of deterministic initial conditions. In particular, we aim to determine some sufficient extra conditions which guarantee that the inequalities remain valid. Using an ODE-approach we prove that the correlation inequalities hold on a small network, i.e. two nodes connected by an edge, even if starting from a mixed initial condition and any edge weight as long as at time $t = 0$ the correlation holds. For a network of three nodes and a general network and by focusing on a specific edge, we give sufficient conditions which guarantee that the correlation inequalities remain valid even for mixed initial conditions. Finally, we show that our approach can be used to prove the result in [7] but only for t close to zero.

It is obvious that the initial condition can be given in such a way that the correlation inequalities are violated even at the initial instant. For example, for a network with two nodes and a single edge, one can set $\langle S_1 I_2 \rangle(0) = 1/2$ and $\langle I_1 S_2 \rangle(0) = 1/2$. This gives $\langle S_1 \rangle(0) = 1/2$, $\langle I_2 \rangle(0) = 1/2$ and $\langle S_1 I_2 \rangle(0) = 1/2$ and hence $\langle S_1 \rangle(0) \langle I_2 \rangle(0) - \langle S_1 I_2 \rangle(0) = -1/4 < 0$. Hence the first, and trivial condition is $\langle S_i \rangle(0) \langle I_j \rangle(0) - \langle S_i I_j \rangle(0) \geq 0$. We will show a simple example below that this condition is not sufficient. In [7] it is assumed that the initial condition is a deterministic state. Starting from a deterministic state we have $\langle S_i \rangle(0) \langle I_j \rangle(0) - \langle S_i I_j \rangle(0) = 0$ for all i and j . We will show below that there is a positive time t^* , such that $\langle S_i \rangle(t) \langle I_j \rangle(t) - \langle S_i I_j \rangle(t) > 0$ for $0 < t < t^*$ when the process starts from a deterministic state. Finally, we show that for certain conditions on the weights we have $\langle S_i \rangle(t) \langle I_j \rangle(t) - \langle S_i I_j \rangle(t) > 0$ for any $0 < t$ starting from any state satisfying $\langle S_i \rangle(0) \langle I_j \rangle(0) - \langle S_i I_j \rangle(0) \geq 0$.

In order to investigate the correlation, the following proposition will be useful.

Proposition 1.

$$\langle S_i \rangle \langle I_j \rangle - \langle S_i I_j \rangle = \langle I_i I_j \rangle \langle S_i S_j \rangle - \langle S_i I_j \rangle \langle I_i S_j \rangle.$$

PROOF. We will use the identities

$$\langle I_i I_j \rangle + \langle S_i S_j \rangle + \langle S_i I_j \rangle + \langle I_i S_j \rangle = 1$$

and

$$\langle S_i \rangle = \langle S_i I_j \rangle + \langle S_i S_j \rangle, \quad \langle I_j \rangle = \langle S_i I_j \rangle + \langle I_i S_j \rangle.$$

Using these we obtain

$$\langle S_i I_j \rangle \langle I_i I_j \rangle + \langle S_i I_j \rangle \langle S_i S_j \rangle + \langle S_i I_j \rangle \langle S_i I_j \rangle + \langle S_i I_j \rangle \langle I_i S_j \rangle = \langle S_i I_j \rangle$$

and

$$\langle S_i \rangle \langle I_j \rangle = \langle S_i I_j \rangle \langle S_i I_j \rangle + \langle S_i I_j \rangle \langle I_i I_j \rangle + \langle S_i S_j \rangle \langle S_i I_j \rangle + \langle S_i S_j \rangle \langle I_i I_j \rangle.$$

Taking the difference of the last two equations yields the desired relation.

□

Before we proceed further we also show a possible ODE-based approach for a single edge, i.e. for $N = 2$, for which system (1)-(5) takes the form

$$\langle \dot{I}_1 \rangle = \tau \langle SI \rangle - \gamma \langle I_1 \rangle, \quad (13)$$

$$\langle \dot{I}_2 \rangle = \tau \langle IS \rangle - \gamma \langle I_2 \rangle, \quad (14)$$

$$\langle \dot{S}I \rangle = -\tau \langle SI \rangle - \gamma \langle SI \rangle + \gamma \langle II \rangle, \quad (15)$$

$$\langle \dot{I}S \rangle = -\tau \langle IS \rangle - \gamma \langle IS \rangle + \gamma \langle II \rangle, \quad (16)$$

$$\langle \dot{II} \rangle = -2\gamma \langle II \rangle + \tau \langle SI \rangle + \tau \langle IS \rangle, \quad (17)$$

$$\langle \dot{S}S \rangle = \gamma \langle SI \rangle + \gamma \langle IS \rangle, \quad (18)$$

where we wrote $\langle XY \rangle$ instead of $\langle X_1 Y_2 \rangle$ for ease of notation.

Proposition 2. *If $\langle II \rangle(0) \langle SS \rangle(0) - \langle SI \rangle(0) \langle IS \rangle(0) \geq 0$, then $\langle II \rangle(t) \langle SS \rangle(t) - \langle SI \rangle(t) \langle IS \rangle(t) \geq 0$ for all $t > 0$ and for arbitrary initial conditions (e.g. deterministic or mixed).*

PROOF. We prove that

$$A(t) = \langle II \rangle(t) \langle SS \rangle(t) - \langle SI \rangle(t) \langle IS \rangle(t)$$

is nonnegative if $A(0) \geq 0$.

Using the differential equations (1)-(5) we can derive a differential equation for the function A as follows.

$$\begin{aligned} \dot{A} &= \langle \dot{II} \rangle \langle SS \rangle + \langle II \rangle \langle \dot{S}S \rangle - \langle \dot{S}I \rangle \langle IS \rangle - \langle SI \rangle \langle \dot{I}S \rangle \\ &= \tau \langle SI \rangle \langle SS \rangle + \tau \langle IS \rangle \langle SS \rangle - 2\gamma \langle II \rangle \langle SS \rangle + \gamma \langle SI \rangle \langle II \rangle + \gamma \langle IS \rangle \langle II \rangle \\ &\quad + \tau \langle SI \rangle \langle IS \rangle + \gamma \langle SI \rangle \langle IS \rangle - \gamma \langle II \rangle \langle IS \rangle + \tau \langle IS \rangle \langle SI \rangle + \gamma \langle IS \rangle \langle SI \rangle - \gamma \langle II \rangle \langle SI \rangle \\ &= \tau (\langle SI \rangle \langle SS \rangle + \langle IS \rangle \langle SS \rangle + 2 \langle SI \rangle \langle IS \rangle) - 2\gamma (\langle II \rangle \langle SS \rangle - \langle IS \rangle \langle SI \rangle) \\ &= -2(\tau + \gamma)A + b, \end{aligned}$$

where

$$b = \tau (\langle SI \rangle \langle SS \rangle + \langle IS \rangle \langle SS \rangle + 2 \langle II \rangle \langle SS \rangle).$$

Thus A satisfies an inhomogeneous linear differential equation. Multiplying this differential equation with $\exp(-2(\tau + \gamma)t)$ and integrating from 0 to t yields

$$A(t)e^{-2(\tau + \gamma)t} - A(0) = \int_0^t b(s)e^{-2(\tau + \gamma)s} ds.$$

The non-negativity of $b(s)$ and $A(0)$ yields that $A(t) \geq 0$ for all nonnegative t .

□

Before studying the statement in the general case, let us introduce the following notation,

$$A_{ij}(t) = \langle S_i \rangle(t) \langle I_j \rangle(t) - \langle S_i I_j \rangle(t) = \langle I_i I_j \rangle(t) \langle S_i S_j \rangle(t) - \langle S_i I_j \rangle(t) \langle I_i S_j \rangle(t), \quad (19)$$

where we have used Proposition 1. For the ease of notation, we will write $\langle XY \rangle$ instead of $\langle X_i Y_j \rangle$ and $\langle I_k XY \rangle$ instead of $\langle I_k X_i Y_j \rangle$ and similarly for $\langle X_i Y_j I_k \rangle$, where the indices i and j are considered to be fixed. Differentiating (19) and using the

differential equations (1)-(5) yield

$$\dot{A}_{ij} = \langle \dot{II} \rangle \langle SS \rangle + \langle \dot{II} \rangle \langle \dot{SS} \rangle - \langle \dot{SI} \rangle \langle IS \rangle - \langle \dot{SI} \rangle \langle \dot{IS} \rangle = Q_1 + Q_2 + \tau \sum_{k=1}^N (g_{jk} Q_{3k} + g_{ik} Q_{4k}), \quad (20)$$

where

$$\begin{aligned} Q_1 &= \gamma(-2\langle II \rangle \langle SS \rangle + \langle SI \rangle \langle II \rangle + \langle IS \rangle \langle II \rangle + \langle SI \rangle \langle IS \rangle - \langle II \rangle \langle IS \rangle + \langle IS \rangle \langle SI \rangle - \langle II \rangle \langle SI \rangle), \\ Q_2 &= \tau g_{ij} \langle SI \rangle \langle SS \rangle + \tau g_{ji} \langle IS \rangle \langle SS \rangle + \tau g_{ij} \langle SI \rangle \langle IS \rangle + \tau g_{ji} \langle IS \rangle \langle SI \rangle \\ Q_{3k} &= \langle ISI_k \rangle \langle SS \rangle - \langle SSI_k \rangle \langle II \rangle - \langle SSI_k \rangle \langle IS \rangle + \langle ISI_k \rangle \langle SI \rangle \\ Q_{4k} &= \langle I_k SI \rangle \langle SS \rangle - \langle I_k SS \rangle \langle II \rangle + \langle I_k SI \rangle \langle IS \rangle - \langle I_k SS \rangle \langle SI \rangle. \end{aligned}$$

Each term will be simplified separately. Simple algebra leads to

$$Q_1 = -2\gamma(\langle II \rangle \langle SS \rangle - \langle IS \rangle \langle SI \rangle) = -2\gamma A_{ij}.$$

The expression for Q_2 can be reduced as follows

$$\begin{aligned} Q_2 &= \tau g_{ij}(\langle SI \rangle \langle SS \rangle + \langle II \rangle \langle SS \rangle - A_{ij}) + \tau g_{ji}(\langle IS \rangle \langle SS \rangle + \langle II \rangle \langle SS \rangle - A_{ij}) \\ &= -\tau A_{ij}(g_{ij} + g_{ji}) + \tau g_{ij} \langle SS \rangle \langle I_j \rangle + \tau g_{ji} \langle SS \rangle \langle I_i \rangle, \end{aligned}$$

where in the last step the identities $\langle II \rangle + \langle SI \rangle = \langle I_j \rangle$ and $\langle II \rangle + \langle IS \rangle = \langle I_i \rangle$ were used.

Based on the identities $\langle SS \rangle + \langle SI \rangle = \langle S_i \rangle$ and $\langle II \rangle + \langle IS \rangle = \langle I_i \rangle$, the term Q_{3k} can be rewritten as

$$Q_{3k} = \langle ISI_k \rangle \langle SS \rangle + \langle ISI_k \rangle \langle SI \rangle - \langle SSI_k \rangle \langle II \rangle - \langle SSI_k \rangle \langle IS \rangle = \langle ISI_k \rangle \langle S_i \rangle - \langle SSI_k \rangle \langle I_i \rangle.$$

Similar transformations lead to

$$Q_{4k} = \langle I_k SI \rangle \langle S_j \rangle - \langle I_k SS \rangle \langle I_j \rangle.$$

Substituting the expressions obtained for Q_1 , Q_2 , Q_{3k} and Q_{4k} into (20) we get

$$\begin{aligned} \dot{A}_{ij} &= -(2\gamma + \tau(g_{ij} + g_{ji}))A_{ij} + \tau g_{ij} \langle SS \rangle \langle I_j \rangle + \tau g_{ji} \langle SS \rangle \langle I_i \rangle \\ &\quad + \tau \sum_{k=1}^N (g_{jk}(\langle ISI_k \rangle \langle S_i \rangle - \langle SSI_k \rangle \langle I_i \rangle) + g_{ik}(\langle I_k SI \rangle \langle S_j \rangle - \langle I_k SS \rangle \langle I_j \rangle)). \end{aligned} \quad (21)$$

This formula yields the solution of the problem for a network with $N = 3$ nodes. Since $g_{ii} = 0$ and $g_{jj} = 0$, the summation for k contains only a single index, when k is different from i and j . For simplicity, we consider the case $i = 1$, $j = 2$ and $k = 3$, use the notation $A = A_{12}$ and $\langle XYZ_k \rangle = \langle XYZ \rangle$. Then (21) takes the form

$$\begin{aligned} \dot{A} &= -(2\gamma + \tau(g_{12} + g_{21}))A + \tau g_{12} \langle SS \rangle \langle I_2 \rangle + \tau g_{21} \langle SS \rangle \langle I_1 \rangle \\ &\quad + \tau g_{23}(\langle ISI \rangle \langle S_1 \rangle - \langle SSI \rangle \langle I_1 \rangle) + \tau g_{13}(\langle SII \rangle \langle S_2 \rangle - \langle SSI \rangle \langle I_2 \rangle). \end{aligned} \quad (22)$$

Now, we can easily show a counter example to the statement. Let $P(SSI) = 1/2$ and $P(SIS) = 1/2$ in the initial state. Then $\langle I_1 \rangle(0) = 0$, $\langle I_2 \rangle(0) = 1/2$ and $\langle S_1 S_2 \rangle(0) = 1/2$. It can be easily seen that $A(0) = 0$ and $\dot{A}(0) = \tau(g_{12} - g_{13})/4$. Hence, $A(t)$ becomes negative when $g_{12} < g_{13}$. On the other hand, if the opposite inequality holds, then $A(t)$ remains positive as it is stated in the following statement.

Proposition 3. *Consider a network with $N = 3$ nodes and the correlation A_{12} . Assume that $g_{12} \geq g_{13}$ and $g_{21} \geq g_{23}$. If $A_{12}(0) \geq 0$, then $A_{12}(t) \geq 0$ for all $t > 0$ and for arbitrary initial conditions.*

PROOF. Using that $\langle SS \rangle \geq \langle SSI \rangle$ the conditions on the weights imply that (22) can be written in the form

$$\dot{A} = -(2\gamma + \tau(g_{12} + g_{21}))A + b,$$

where b is nonnegative. Then using the same idea as in the proof of Proposition 2, we get that $A_{12}(t) \geq 0$ for all $t > 0$.

□

Note that this means that, in a triangle with equal weights, $S - I$ pairs remain non-negatively correlated if they are non-negatively correlated initially, and this is true not only for deterministic initial conditions.

Similar proof, using (21), leads to the following statement.

Proposition 4. *Consider the edge (i, j) in a network with N nodes and the correlation A_{ij} . Assume that $g_{ij} \geq \sum_{k=1}^N g_{ik}$ and $g_{ji} \geq \sum_{k=1}^N g_{jk}$. If $A_{ij}(0) \geq 0$, then $A_{ij}(t) \geq 0$ for all $t > 0$ and for arbitrary initial conditions.*

Finally, we can turn to the case of deterministic initial condition. It can be easily seen that $A_{ij}(0) = 0$, for these initial conditions and (21) shows that $\dot{A}_{ij}(0) = 0$ also holds. Differentiating (21) once more, one obtains that $\ddot{A}_{ij}(0) > 0$. This implies that $A_{ij}(t) > 0$ for small enough values of t . This proves the following theorem.

Theorem 4.1. *Let $\langle S_i \rangle$, $\langle I_j \rangle$ and $\langle S_i I_j \rangle$ solve system (1)-(5). If we start from a deterministic initial condition, then there exist a positive time t^* , such that $\langle S_i \rangle(t) \langle I_j \rangle(t) - \langle S_i I_j \rangle(t) \geq 0$ holds for all $0 < t < t^*$.*

5. Analysis of the closed model. The goal in this section is to analyse system (7) from the dynamical systems point of view. The closure W satisfies the conditions in Definition 2.1, moreover, according to the second inequality in (8) it satisfies $W(x, y) \geq xy$ as well. Thus our aim here is to understand the dynamical behaviour of system (7) when W satisfies

$$xy \leq W(x, y) \leq \min(x, y) \text{ for all } x, y \in [0, 1]. \quad (23)$$

The lower bound $W(x, y) = xy$ is covered in [16], and this result is presented first.

Theorem 5.1. *Given a directed, weighted, and strongly-connected network, G , let $\Lambda_{\max}(G)$ be the largest eigenvalue of the adjacency matrix of G . Let the closure in (7) be given as $W(x, y) = xy$. If $\gamma < \tau \Lambda_{\max}(G)$, then a unique endemic (nonzero) steady state exists, and it is stable. Moreover, all of its coordinates are positive. If $\gamma > \tau \Lambda_{\max}(G)$, then there is no endemic steady state and the disease-free steady state is stable.*

Concerning the upper bound $W(x, y) = \min(x, y)$, the following result can be easily proved.

Proposition 5. *Let G be a directed and weighted network and let the closure in (7) be given as $W(x, y) = \min(x, y)$. Then the only steady state is the disease-free one and it is stable.*

PROOF. Assume that $x^* \in [0, 1]^N$ is a steady state, that is for all i we have

$$\tau \sum_{j=1}^N g_{ij}(x_j^* - \min(x_i^*, x_j^*)) - \gamma x_i^* = 0.$$

Let x_i^* be (one of) the greatest coordinate of the steady state. Then for all j we have $x_j^* - \min(x_i^*, x_j^*) = 0$, hence the coefficient of τ in the above equation is zero, implying that $x_i^* = 0$. Since $0 \leq x_j^* x_i^* = 0$ for all j , we get that $x^* = 0$, that is the only steady state is the disease-free one. This reasoning also shows that the largest coordinate of a solution has negative derivative, which implies the stability of the disease-free steady state. \square

Thus a transcritical bifurcation occurs when the closure is $W(x, y) = xy$ and there is no bifurcation when $W(x, y) = \min(x, y)$; that is the threshold behaviour disappears when such a crude closure is used. This however raises the question of studying the intermediate regime when W is between the two extremes. Below we give a sufficient condition on closures to ensure that the threshold behaviour is maintained.

We will consider closures where W satisfies

$$xy \leq W(x, y) \leq xy + V(x, y) \min(x, y) \text{ for all } x, y \in [0, 1], \quad (24)$$

where $V : [0, 1]^2 \rightarrow [0, r]$, with some $r \in (0, 1)$, is a continuous function satisfying $V(0, 0) = 0$ and $xy + V(x, y) \min(x, y) \leq \min(x, y)$. We note that the inequalities in (24) yield a sufficient condition for the existence of the transcritical bifurcation. This means that it may be possible to identify closures that lead to transcritical bifurcation but do not satisfy condition (24).

We note that $W(x, y) = xy$ obviously satisfies this condition with $V(x, y) = 0$, and a non-trivial example is $W(x, y) = \sqrt{xy} \min(\sqrt{x}, \sqrt{y})$. For the latter, simple calculation shows that there exists a $V(x, y)$ such that this is positive and bounded by a constant $r < 1$. Below we will prove that for any choice of W that satisfies condition (24) the same threshold as in Theorem 5.1 is obtained.

The non-trivial steady state $x \in (0, 1]^N$ of system (7) is given by

$$\gamma x_i = \tau \sum_{j=1}^N g_{ij}(x_j - W(x_i, x_j))$$

that will be rearranged using $x_j - W(x_i, x_j) = x_j - x_i x_j + x_i x_j - W(x_i, x_j)$ as

$$x_i(\alpha + (Gx)_i) = (Gx)_i - F_i(x), \quad (25)$$

where $\alpha = \gamma/\tau$, $(Gx)_i$ is the i -th coordinate of the vector Gx and

$$F_i(x) = \sum_{j=1}^N g_{ij}(W(x_i, x_j) - x_i x_j).$$

Expressing x_i from (25) we get the fixed point equation $x = T(x)$ for the non-trivial steady state with

$$T_i(x) = \frac{(Gx)_i - F_i(x)}{\alpha + (Gx)_i}. \quad (26)$$

We can immediately see that T maps the unit hypercube $[0, 1]^N$ into itself and the origin is its fixed point, representing the disease-free steady state. We will show that in the case $\gamma < \tau\Lambda$, that is $\alpha < \Lambda$, T has a nontrivial fixed point in the interior of the hypercube, representing an endemic steady state. (Here $\Lambda = \Lambda_{\max}(G)$ is the largest eigenvalue of the adjacency matrix of G .) The existence of this fixed point will be verified by using Brouwer's fixed point theorem on a suitably chosen convex subdomain of the hypercube not containing the origin. In order to achieve this goal we will need a few auxiliary results.

Proposition 6. *For a directed, weighted, and strongly-connected network, given by its adjacency matrix G , there exists a positive number μ , for which the following holds. If $(Gx)_i < \eta$ and $x_i \geq 0$ for all $i = 1, 2, \dots, N$, then $|x| < \mu\eta$.*

PROOF. Since the network is strongly connected every column of G contains at least one nonzero entry. Hence $Gx \neq 0$ once $x_i \geq 0$ for all $i = 1, 2, \dots, N$ and $x \neq 0$. Therefore

$$m = \min\{|Gx| : x_i \geq 0, |x| = 1\} > 0.$$

If $(Gx)_i < \eta$ for all $i = 1, 2, \dots, N$, then $|Gx| < \eta\sqrt{N}$. On the other hand, $|Gx| = |x| \left| G \frac{x}{|x|} \right| > m|x|$, implying $m|x| < \eta\sqrt{N}$. Hence the statement holds with $\mu = \sqrt{N}/m$.

□

For the next proposition we introduce a function, $h : [0, +\infty) \rightarrow [0, 1)$, which is defined by

$$h(z) = \frac{z}{\alpha + z}.$$

Proposition 7. *For any $\beta < 1/\alpha$ there is a $\omega > 0$, such that $h(z) < \omega$ implies $\beta z < h(z)$, when $z \neq 0$.*

PROOF. One can easily check that $h(0) = 0$, $h'(0) = 1/\alpha$, $h'(z) > 0$ and $h''(z) < 0$ for all $z \geq 0$, i.e. h is increasing and concave. Hence a line with slope $\beta < h'(0)$ passing through the origin, lies below the graph of h in a sufficiently short interval $(0, z_0)$. Then the statement holds with $\omega = h(z_0)$.

□

Proposition 8. *For any $x \in [0, 1]^N$ we have $T_i(x) \geq (1 - r)h((Gx)_i)$.*

PROOF. According to (24) we have $W(x_i, x_j) \leq x_i x_j + r x_j$, hence

$$\sum_{j=1}^N g_{ij}(r x_j + x_i x_j - W(x_i, x_j)) \geq 0$$

yielding $r(Gx)_i \geq F_i(x)$, that is $(Gx)_i - F_i(x) \geq (1 - r)(Gx)_i$. Therefore (26) leads to

$$T_i(x) \geq \frac{(1 - r)(Gx)_i}{\alpha + (Gx)_i} = (1 - r)h((Gx)_i).$$

□

Proposition 9. *Let $\alpha < \Lambda$. Then there is a $\rho > 0$, such that $T_i(x) < \rho$ for all i implies $(Gx)_i < \Lambda T_i(x)$, when $(Gx)_i \neq 0$.*

PROOF. Choose a small positive ε , for which $\Lambda(1 - \varepsilon) > \alpha$ and introduce $\beta = 1/\Lambda(1 - \varepsilon) < 1/\alpha$. Choose ω to β according to Proposition 7. Choose a positive δ to ε according to the continuity of V given in (24), that is $|V(x, y)| < \varepsilon$, when $|x|, |y| < \delta$. Finally, determine $\kappa > 0$ from

$$\mu\alpha \frac{\kappa}{1 - \kappa} = \delta,$$

where μ is given in Proposition 6. Now we show that choosing a positive ρ satisfying

$$\rho < \omega(1 - \varepsilon), \quad \rho < \kappa(1 - r)$$

the statement holds.

Using Proposition 8, we get for any i that

$$\kappa(1-r) > \rho > T_i(x) \geq (1-r)h((Gx)_i).$$

Simple algebra shows that $\kappa > h((Gx)_i)$ implies $(Gx)_i < \alpha\kappa/(1-\kappa)$. Hence, according to Proposition 6, we have $|x| < \mu\alpha\frac{\kappa}{1-\kappa} = \delta$. The choice of ε ensures that $W(x_i, x_j) - x_i x_j \leq \varepsilon x_j$, hence

$$F_i(x) \leq \sum_{j=1}^N g_{ij}\varepsilon x_j = \varepsilon(Gx)_i.$$

Therefore (26) leads to

$$T_i(x) \geq \frac{(1-\varepsilon)(Gx)_i}{\alpha + (Gx)_i} = (1-\varepsilon)h((Gx)_i).$$

Now,

$$\omega(1-\varepsilon) > \rho > T_i(x) \geq (1-\varepsilon)h((Gx)_i).$$

According to Proposition 7, we get that $h((Gx)_i) > \beta(Gx)_i$, hence

$$T_i(x) \geq (1-\varepsilon)h((Gx)_i) > (1-\varepsilon)\beta(Gx)_i = \frac{1}{\Lambda}(Gx)_i,$$

and this completes the proof.

□

Now we are ready to prove the existence of the endemic steady state and the presence of a transcritical bifurcation.

Theorem 5.2. *Given a directed, weighted, and strongly-connected network, G , let Λ be the largest eigenvalue of the adjacency matrix of G . Let the closure W in (7) satisfy (24). If $\gamma > \tau\Lambda$ then the origin is the only steady state of the system. In the case $\gamma < \tau\Lambda$, an endemic (nonzero) steady state also exists.*

PROOF. We first consider the $\gamma > \tau\Lambda$ case and take a steady state $x \in [0, 1]^N$. According to (25) and using that F_i is nonnegative we get

$$\gamma x_i \leq \tau(1-x_i)(Gx)_i \leq \tau(Gx)_i.$$

It is easy to see that for two vectors, u and v with nonnegative coordinates, the inequality $0 \leq u_i \leq v_i$ for all i implies $|u| \leq |v|$. Hence for any nonzero steady state $x \in [0, 1]^N$ we have

$$\gamma|x| \leq \tau|G(x)| \leq \tau\Lambda|x| < \gamma|x|,$$

where we used that Λ is the largest eigenvalue of G . Hence there is no endemic steady state. We note that this part of the proof only used the fact that $W(x, y) \geq xy$, condition (24) has not been used.

Let us turn to the case $\gamma < \tau\Lambda$. As we mentioned above, we will prove the existence of the endemic steady state by applying Brouwer's fixed point theorem to the mapping T given in (26) in a suitably chosen domain. The goal is to exclude the origin from this domain, hence we introduce a half-space $S = \{x \in \mathbb{R}^N : \langle x-a, u \rangle \geq 0\}$ with some appropriately chosen vectors $a, u \in \mathbb{R}^N$. Then our domain will be $\Omega = [0, 1]^N \cap S$. In order to have a nonempty intersection we will choose a from the hypercube $[0, 1]^N$ and u will be the unique positive eigenvector of G corresponding to the maximal eigenvalue Λ , that is $Gu = \Lambda u$.

In order to prove the invariance of the domain Ω it is useful to determine the intersection points of the hyperplane given by $\langle x-a, u \rangle = 0$ and the coordinate axes. The intersection point on the i -th axis is at $c_i = \langle a, u \rangle / u_i$. It is easy to see

that a point $y \in [0, 1]^N$ is in Ω if there is a coordinate i , for which $y_i \geq c_i$. Namely, if $y \in [0, 1]^N$ is not in Ω , then $\langle y, u \rangle < \langle a, u \rangle = c_i u_i$ for all i , hence $y_i u_i < c_i u_i$ leading to $y_i < c_i$ for all i . Now, choose $a \in [0, 1]^N$ in such a way that for all i we have $c_i < \rho$ given in Proposition 9, that is $\langle a, u \rangle / u_i < \rho$ for all i .

We will prove that T maps Ω into itself. We know that T maps to $[0, 1]^N$, hence we only need to prove that $\langle T(x) - a, u \rangle \geq 0$ holds for any $x \in \Omega$. We have previously shown that, if there is an index i for which $T_i(x) \geq \rho$, then $T(x) \in \Omega$. Hence we only need to consider the case when $T_i(x) < \rho$ for all i . In this case we can apply Proposition 9 yielding $T_i(x) > (Gx)_i / \Lambda$. Hence $T_i(x) u_i > (Gx)_i u_i / \Lambda$, leading to

$$\begin{aligned} \langle T(x), u \rangle &= \sum_{i=1}^N T_i(x) u_i > \frac{1}{\Lambda} \sum_{i=1}^N (Gx)_i u_i = \frac{1}{\Lambda} \sum_{i=1}^N u_i \sum_{j=1}^N g_{ij} x_j \\ &= \frac{1}{\Lambda} \sum_{j=1}^N x_j \sum_{i=1}^N g_{ij} u_i = \frac{1}{\Lambda} \sum_{j=1}^N x_j (Gu)_j = \frac{1}{\Lambda} \sum_{j=1}^N x_j \Lambda u_j = \langle x, u \rangle \geq \langle a, u \rangle. \end{aligned}$$

Thus we proved $\langle T(x) - a, u \rangle \geq 0$, which proves that T maps the convex, compact domain Ω into itself, hence by Brouwer's fixed point theorem it has a fixed point in Ω , which is a nontrivial steady state completing the proof of the theorem.

□

We note that the stability of the steady states was also determined in the special case $W(x, y) = xy$. Further conditions on the smoothness of W would make it possible to generalise the stability result of Theorem 3.8 in [12] for different choices of W .

6. Discussion. In Section 4 we proved that the closure $W(x, y) = xy$ satisfies the second assumption of Theorem 3.2, that is this closure leads to an upper bound of the exact model. Similarly, in Theorem 3.3 we have shown that $W(x, y) = \min(x, y)$ yields a lower bound of the exact model. However, further work could focus on finding more accurate upper and lower bounds with the possibility of constructing a sequence of closures whose limit is closer in some sense to the exact model.

The analysis of the closed model was presented in Section 5. However, the investigation of the local and global stability for a general closure relation is still an open question. Moreover, we have shown that the qualitative behaviour of the closed system depends on the closure and can be significantly different: it may or may not lead to a transcritical bifurcation. The question of whether a closed system shares the same qualitative features as the exact model is an important one, and ideally the behaviour of the two systems should remain the same. Thus identifying the closure or closures which separate different regimes, those that conserve the qualitative behaviour of the exact system versus those that do not, remains an important direction for further research. One possible step towards achieving this may be to find closures that delimit closed models that have different qualitative behaviour when compared to each other, without considering their relation to the exact model.

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